SPECTROSCOPIC AND THEORETICAL CONSIDERATIONS OF CYCLOPROPENONE

BY

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ABSTRACT

The absorption spectrum of cyclopropenone has been photographically recorded under conditions of long pathlength (60 m), and moderate resolution (7.8 Å/mm). The absorption was assigned to the electron promotion, n --> π^* (C=O), and to the electronic transition $\tilde{B}^1A_2$ -- $\tilde{X}^1A_1$. The spectrum proved to be limited in band structure, which hindered the vibrational assignment. Structures and vibrational frequencies were calculated for the $\tilde{X}^1A_1$, $\tilde{a}^3B_1$, and $\tilde{b}^3A_2$ states at the 6-31g* Hartree-Fock level. The calculations confirmed the assigned transition and predicted the position and structure of the second $\tilde{a}^3B_1$ system.